

NCCS – Getting Started

NCCS User's Meeting February 14, 2006



Robert Whitten Jr.

User Assistance Group

National Center for Computational Sciences

Oak Ridge National Laboratory

OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY



Outline

- **Introduce the stars**
- **Support options**
- **Common features**
- **Managing your allocations**
- **Future directions**
- **X1E overview (Richard Mills)**
- **XT3 overview (Bronson Messer)**

Jaguar - Cray XT3

- **5294 Nodes**
- **2.4Ghz AMD opteron**
- **25TF**
- **Lustre filesystem**
- **Unicos/lc**
 - Linux/Catamount
- **10th fastest computer**
 - www.top500.org



Phoenix - Cray X1E

- **1024 MSPs**
- **Custom vector processors**
- **18TF**
- **Largest X1E**
- **Linux cross compiler**
 - robin.ccs.ornl.gov



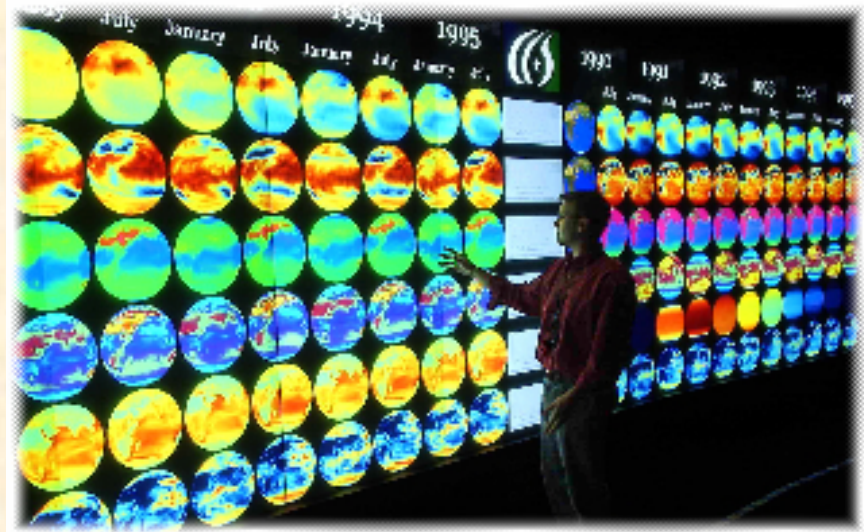
Ram - SGI Altix

- **256 Intel Itanium2 processors**
- **2TB shared memory**
- **LCF pre/post processing**



Hawk - visualization cluster

- **64 node Linux cluster**
 - Everest – 14 nodes
 - Render – 50 nodes
- **Quadrics Elan3 interconnect**
- **27 panel powerwall**
- **35 million pixel resolution**



OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY



HPSS – Mass Storage

- **Tape and disk storage**
- **Suitable for backup and long term storage**
- **900TB capacity today**
- **Expandable to 1.7PB**
- **hsi to access**
 - **FTP-like**

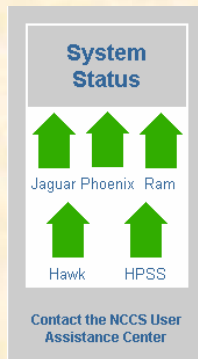


How to get help:

- **Web (www.nccs.gov)**
 - System status
 - FAQs
 - Available software
- **Email (help@nccs.gov)**
 - User Assistance Center
 - M-F 9am-5pm ET
- **Phone (865-241-6536)**
 - 24/7

Web support

- System Status
- Resource Info
- Available software



Phoenix

Phoenix is a Cray X1E provided as a primary system in the National Center for Computational Sciences (NCCS).

Jaguar

Jaguar is a Cray XT3 provided as a primary system in the National Leadership Computing Facility (NLCF).

The current Jaguar installation has 5294 nodes, each with a 2.4-GHz AMD Opteron processor and 2 GB of memory. 5212 nodes are available in the compute partition, and the remainder provide I/O and login services.

Each node is connected to a Cray Seastar router through Hypertransport, and the Seastars are all interconnected in a 3D-torus topology. The resulting interconnect has very high bandwidth, low latency, and extreme scalability.

The operating system is UNICOS/lc, which is a combination of Linux on the service nodes and the Catamount microkernel on the compute nodes. Catamount is designed to minimize system overhead, thus allowing scalable low-latency global communication.

External Links:

- Cray XT3 Overview at Cray, Inc.
- Red Storm, the project between Cray and Sandia National Laboratories that led to the XT3 product.

- Open Issues
- C/C++
- Fortran
- File Systems
- Batch Jobs
- Interactive
- System Status

Libraries

	version	jaguar	phoenix	ram	hawk
ATLAS					
AZTEC					
BLACS					
BLAS					
FFTW					
Global					
HDF5					

Applications and Tools

	version	jaguar	phoenix	ram	hawk
CDAT	4.0b4			x	
Cg	1.4.0-4				x
Ensign	7.6.4			x	
GAMSS	jan2004			x	
gdb	5.0		x		
	5.3.90	x			
	6.1			x	
	version	jaguar	phoenix	ram	hawk
gmake	3.7.9		x	x	
	3.8.0	x			
Grace	4.1.18			x	
Histx	1.2a			x	
Ncarg	4.3.1			x	
	4.4.1		x		

OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY



Email support

- **help@nccs.gov**
- **RT system**
 - Automated response
- **Help us help you**
 - Username
 - Description
 - Machine
 - Error messages
- **More is better**

Dear NCCS User,

This is an automated response to your NCCS support inquiry. This issue has been assigned ticket #14516. If you wish to add more information to this ticket, simply reply to this message without modifying the subject line. To report a separate issue, email help@nccs.gov with a new subject.

For the fastest possible response, make sure your ticket includes your user name, the system name(s) and the location of any executables, scripts, and output files related to the error. For batch jobs, please include the job number.

Information including scheduled outages, system availability, FAQs, and current system issues can be found at <http://info.nccs.gov>.

The NCCS User Assistance Center is staffed Monday through Friday from 9:00 AM to 5:00 PM Eastern Time.

NCCS User Assistance Center
National Center for Computational Sciences
Oak Ridge National Laboratory
help@nccs.gov 865-241-6536

Phone support

- **24/7 support**
- **Staffed by UAG & CompSci**
 - M-F 9am-5pm ET
- **865-241-6536**



Common features

- **NFS mounted home directory**
 - 500MB quota
- **Scratch space**
 - Temporary
 - /tmp/work/<username>
- **Access to HPSS**
- **One time password access**
- **Totalview**

Connecting

- **Use Secure Shell**
 - `ssh userid@<machine>.ccs.ornl.gov`
 - `ssh user@phoenix.ccs.ornl.gov`
- **One time password**
 - RSA SecurID
 - **PASSCODE = PIN + Token Code**
 - SSH client need keyboard-interactive
- **Jaguar is different**
 - `ssh user@home.ccs.ornl.gov` then –
 - `ssh user@jaguar.ccs.ornl.gov`



Modules

- **Quick and easy environment setup**
- **Commands**
 - module list
 - module avail
 - module load <module>
 - module unload <module>
 - module swap <old> <new>
 - module help
- **Example**
 - module load craytools

Tips

- **Home directory quota 500MB**
 - Use scratch space - /tmp/work/<user>
- **Use *lsquota* to determine disk quota**
- **HPSS works best with >1GB files**
 - tar cvf - . | hsi put - : data.tar
- **Need software installed?**
 - help@nccs.gov

Accounting

- **Every project has an identifier**
 - FUSXXX, CHMYYYzzz, etc
- **Include in PBS scripts**
 - #PBS –A FUS123
- **No identifier = no submission**
- **Aids in proper accounting of allocations**

Managing Allocations

- **Adding access or users**
 - <https://secure.ccs.ornl.gov/request.new.html>
 - Has everyone turned in Appendix B???
- **Subprojects**
- **Allocation reports**
 - Weekly for primary investigators
- **Project wiki space available**
 - By request
 - users.nccs.gov/<projectID>

The Horizon

- **Web access to accounting information**
- **User satisfaction surveys**
- **Periodic reports**
- **Highlights**

How can we help you?

- **Suggestions encouraged**
 - **help@nccs.gov**